Recombination in Semiconductors: Appearance of Non-equilibrium Carriers due to Injection or Redistribution in the Sample

I. N. Volovichev,* G. Espejo,[†] and Yu. G. Gurevich.[‡] Departamento de Física, CINVESTAV—I.P.N., Apdo. Postal 14-740, México, D.F. 07000, México

O. Yu. Titov§

CICATA—I.P.N., José Siurob No. 10,

Col. Alameda, C.P. 76040,

Santiago de Querétaro, Qro., México

A. Meriuts

Kharkov Polytechnic University, 21 Frunze Str., Kharkov 310002, Ukraine (Dated: February 1, 2008)

It is shown that the traditional approach for consideration of recombination under condition of steady-state current in the absence of external carrier generation is internally contradictory. Sometimes the approach leads to obviously incorrect results. Such situations are demonstrated and a new method for consideration of recombination is proposed.

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In the present paper we would like to consider some internal inconsistencies in the conventional description when we have carrier recombination under condition of steady-state current. Practically all text-books^{1,2,3,4,5} present technique to solve the given problem based on the solution of a set of continuity equations:

$$\operatorname{div}\mathbf{j}_n = eR_n, \quad \operatorname{div}\mathbf{j}_p = -eR_p$$

where n and p are the electron and hole concentration, $\mathbf{j}_{n,p}$ are the current of electrons and holes, $R_{n,p}$ are the electron and hole recombination rate respectively. Here we consider the absencess of external generation of carriers (by light, etc.). Thus the nonequilibrium carriers are a result of injection or accumulation of carriers near potential barriers at interfaces. For small concentration of non-equilibrium carriers $\delta n \equiv n - n_0 \ll n_0$, $\delta p \equiv p - p_0 \ll p_0$ (where n_0 , p_0 are concentration of electrons and holes without the current) the recombination rates are widely assumed to be of the following form:

$$R_n = \frac{\delta n}{\tau_n}, \qquad R_p = \frac{\delta p}{\tau_p},$$
 (1)

where τ_n , τ_p are life times of electrons and holes respectively.

Obviously, by virtue of charge preservation law an extra condition

$$R_n = R_n \tag{2}$$

should hold. Although it is not mentioned in the literature that Eq. (2) makes the system overdetermined. Some authors³ use the latter expression as an equation to find the carrier concentration or to reduce by one the number of unknowns in the problem. However, such approach seems to be incorrect because the Eq. (2) is not a new condition for the concentration of non-equilibrium carriers, rather it is the criterion for correctness of the recombination description, and should fulfill identically at any concentration of non-equilibrium carriers. Probably due to this reason other approach frequently is used, ^{1,2,3,4,5,6,7} assuming

$$R_n \equiv R_p = \frac{\delta p}{\tau_p},\tag{3}$$

where δp means the non-equilibrium concentration of minority carriers. Just this approach is classical and is used widely both in text-books, and in papers devoted to kinetic phenomena in semiconductors.

This description possesses a serious inconsistency. It becomes especially obvious if we consider injection of majority carriers. From physical reasons it is evident: injected non-equilibrium majority carriers should recombine. While from a formal point of view, as far as non-equilibrium minority carriers do not occur ($\delta p = 0$) the recombination rates are

also equal to zero $R_n = R_p = 0$. Below we consider more cases, when the conventional description of a recombination is unacceptable.

Elimination of the given inconsistency is not complicated and can be based on the well known formulas presented in the above mentioned text-books. It is easy to get the following expressions for recombination processes³ by a sequential statistical consideration of transitions between valence and conduction bands and between the bands and impurity levels (if they are present):

$$R_n = R_p = \alpha (np - n_i^2) \tag{4}$$

for interband recombination and

$$R_n = R_p = \frac{np - n_i^2}{\tau_n^0(p + p_1) + \tau_n^0(n + n_1)}$$
(5)

for recombination through an impurity level according to the Shockley-Read model.⁸

Here α is the recombination factor, n_i is the carrier concentration of the intrinsic semiconductor, $\tau_{n,p}^0$, n_1 , and p_1 are characteristics of the impurity level.

We should emphasize once again that the equality $R_n = R_p$ is inherent in correct model and holds identically, not causing overdetermination of the system.

Linearizing these expressions for the case of weak deviation from the condition of thermodynamic equilibrium (the changes of carrier concentrations due to current are small on comparison with their equilibrium values), we have for both cases:

$$R_n = R_p = \frac{\delta n}{\tau_n} + \frac{\delta p}{\tau_p}, \quad \text{with } \frac{\tau_n}{\tau_p} = \frac{n_0}{p_0}.$$
 (6)

Just these expressions, being used in Eqs. (1), eliminate all mentioned above inconsistencies.

Also let us pay attention to another aspects of the problem. As it is easy to notice from Eqs. (6), in bipolar semiconductors generally it is impossible to introduce correctly a life time of carriers concept. An exception is the case of quasineutrality when $\delta n = \delta p$ and the introduction of unified life time of carriers $\tau^{-1} \equiv \tau_n^{-1} + \tau_p^{-1}$ becomes possible. In the absence of quasineutrality it is plausible to speak about life time of carriers and to use the conventional approach Eq. (3) only if $(\delta n/\delta p) \ll (\tau_n/\tau_p) = (n_0/p_0)$ (here, as it was mentioned above, n means concentration of majority carriers). Naturally, the fulfilment of this condition is not a priori obvious.

Let us notice that another baseless idea is widespread, namely presence of only interband recombination is sufficient condition for the equality $\delta n = \delta p$ to be fulfilled.^{1,3,4} But there is no proof for this conclusion, and moreover, a case of injection obviously contradicts it.

Thus, in general case for static current either it is impossible to introduce correctly the concept of life time or life times are the same for both electrons and holes.

For the sake of justice we should notice, that as a rule in the literature either injection phenomena⁷ (when linearized equations are not valid due to high concentration of non-equilibrium carriers) or just the quasineutrality approach are considered. From our point of view, it is just the only explanation why so internally contradictory method to describe kinetic phenomena with the presence of recombination is widely used in many text-books and monographies.

Similar problem arises for description of a surface recombination. Correct expression for it should be obtained from consideration of transitions between the bands and impurity levels both inside the semiconductor, and between bands of different semiconductors (or between bands of the semiconductor and metal in case of a metal-semiconductor contact). The correct expression for the surface recombination rate should ensure identical equality of electron and hole recombination rates at any concentration of non-equilibrium carriers at the contact (as in case of volume recombination). It is obvious that in general case the expression of the following form meets the requirement:

$$S = s_n \delta n + s_p \delta p, \tag{7}$$

where coefficients $s_{n,p}$ should be obtained from microscopic consideration of corresponding transitions.

Some authors use that formula at initial stage of calculations, then giving it up and proceeding to the traditional (but incorrect!) expression $S_n = s_n \delta n$, $S_p = s_p \delta p$. Rather characteristic consideration is presented in Ref. 6, where quasilevels of electrons and holes are assumed to coincide. That, in its turn, implicitly presumes infinite surface (or volume) recombination rate.

The situation becomes more complicated, if there is an inhomogeneous temperature distribution (temperature field) in the semiconductor. It is problematic to choose a concentration which can be considered as a level of reference of non-equilibrium concentration (for example, which one should be taken as the reference: $n_0(T_0)$, $n_0[T(x)]$, $n_0[\overline{T}(x)]$, etc). A way out from this position can be found by successive consideration of process of establishment of "equilibrium"

(or in constancy of electrochemical potential in the sample) in the circuit. ¹⁰ Evidently, this method is acceptable only if the temperature field is given. Other, universal and more simple, from our point of view, way to solve this problem is to return to statistical consideration of transitions of carriers between bands and impurity levels in the presence of temperature field. In this case the value of concentration in thermodynamic equilibrium (in the absence of the temperature gradient) or the values corresponding to the mean temperature of the sample can be accepted as the reference level of concentration (i.e. n_0 and p_0). This method works as well in the case, when the temperature field should be determined self-consistently.

Thus for interband recombination we come back to expressions (4), where the values α and n_i are functions of temperature ($\alpha = \alpha[T(x)]$, $n_i = n_i[T(x)]$). For small deviation from the equilibrium state (after linearization) we receive the following expressions for volume recombination rate in the temperature field:

$$R_n = R_p = \frac{\delta n}{\tau_n} + \frac{\delta p}{\tau_p} + \gamma \delta T, \tag{8}$$

where $\gamma \equiv (1/2\tau)(\partial n_i/\partial T)$; $\delta T \equiv T - T_0$; T_0 is the equilibrium temperature (above-mentioned reference level of temperature). Let us note that in the approximation of small nonequilibrium carrier concentrations ($\delta n \ll n_0$, $\delta p \ll p_0$) thermal dependence of the recombination factor α does not manifest itself.

Thus, the presence of a temperature gradient results in appearance of an additional term in expressions for recombination rates. This term takes into account the change of the rate of thermal generation (which, as it is well known, is proportional to squared concentration of intrinsic semiconductor at given temperature). As far as we know, anywhere but Ref. 10, this contribution has not been taken into account in consideration of thermoelectric phenomena.

Finally, if there is no unified temperature of carriers and phonons (for example, hot electrons situation³), it is easy to prove by a similar way that one more term appears in the expressions for recombination rates. It proportional to the heating of carriers:¹¹

$$R_n = R_p = \frac{\delta n}{\tau_n} + \frac{\delta p}{\tau_p} + \gamma (T(x) - T_0) + \beta (T_e - T_0),$$
 (9)

where T_e is the temperature of hot electrons, T(x) is assumed to be the lattice temperature. The coefficient β depends on concentration of carriers, the lattice temperature and capture factor of carriers by the impurity level (or corresponding value for interband recombination).

Let us note that a coordinate dependence of electron temperature $T_e = T_e(x)$, that is a general case, does not affect the term $\gamma(T(x) - T_0)$ from Eq. (9), which is the same as in Eq. (8). This is due to the fact that this term describes thermal generation of carriers, which can not be influenced by population of the conduction band (i.e. by electron temperature) just because of huge concentration of free states in the conduction band.

Thus, we would like to pay attention of researchers to the fact, that holding a firm place approach to the description of a recombination in steady-state mode is internally contradictory and in many cases, especially common to modern problems, its hasty application can lead to incorrect results. We would like to mention, as an example, thin-film devices, where it is easy to disturb the quasineutrality and to generate essential gradients of temperature and energy nonequilibrium of carriers due to carriers heating by an applied field.

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^{*} Permanent address: Institute for Radiophysics and Electronics, National Academy of Sciences of Ukraine, Kharkov 310085, Kharkov 310085, Ukraine.

[†] Electronic address: gespejo@fis.cinvestav.mx

[‡] Electronic address: gurevich@fis.cinvestav.mx

[§] Electronic address: oleg.titov@aleph-tec.com

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